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A modification of Gauss-Newton method for nonlinear least squares problems

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1 Introduction

In this paper, we consider numerical methods for minimizing a sum of squares of nonlinear functions

$$(1.1) \quad f(x) = \frac{1}{2} \|r(x)\|^2,$$

where $m \geq n$, $r(x) = (r_1(x), \dots, r_m(x))^T$, $r_j : R^n \rightarrow R$ are twice continuously differentiable for $j = 1, \dots, m$, and $\| \cdot \|$ denotes the l_2 norm. We will denote by x_* a local minimizer. This type of problem is among the most commonly occurring and important applications of nonlinear optimization.

Gradient methods are usually used for solving this problem. A prototype algorithm of gradient methods is formed as follows:

[GRAD]

Step 0. Given an initial guess $x_0 \in R^n$. Set $k = 0$.

Step 1. If $\|\nabla f(x_k)\|$ is very small, then stop. Otherwise, go to Step 2.

Step 2. Construct a matrix $B_k \in R^{n \times n}$.

Step 3. Obtain a search direction d_k by solving the linear system of equations

$$(1.2) \quad B_k d = -\nabla f(x_k).$$

Step 4. Set $x_{k+1} = x_k + \alpha_k d_k$ for some suitable step size $\alpha_k > 0$.

Step 5. Set $k = k + 1$ and go to Step 1. \square

Setting

$$B_k = \nabla^2 f(x_k) = J(x_k)^T J(x_k) + \sum_{j=1}^m r_j(x_k) \nabla^2 r_j(x_k)$$

in the algorithm [GRAD], we have Newton's method. Since the complete Hessian matrix is often expensive to compute, methods have been developed which use only the first derivative information. Setting $B_k = J(x_k)^T J(x_k)$ in the algorithm [GRAD], we have

the Gauss-Newton method. This method finds a search direction d_k by solving the linear system of equations

$$(1.3) \quad J(x_k)^T J(x_k) d = -J(x_k)^T r(x_k).$$

We know that the Gauss-Newton method performs very well for zero residual problems but does not for large residual problems. In other words, the matrix $J(x_k)^T J(x_k)$ is a good approximation to the Hessian matrix near the solution for zero residual problems but is not for the large residual problems. The poor performance of the Gauss-Newton method for large residual problems is caused by neglecting the second part of the Hessian matrix $\nabla^2 f(x)$. In order to overcome this difficulty, the structured quasi-Newton method was proposed [3]. This method approximates the second part $\sum_{j=1}^m r_j(x_k) \nabla^2 r_j(x_k)$ by some matrix A_k and produces a search direction d_k by solving the linear system of equations

$$(1.4) \quad (J(x_k)^T J(x_k) + A_k) d = -J(x_k)^T r(x_k).$$

A matrix A_k is generated by updating the previous approximation A_{k-1} based on the idea of the secant method. As a secant condition, Dennis [2] proposed the condition

$$(1.5) \quad A_k s_{k-1} = q_{k-1}$$

with

$$(1.6) \quad s_{k-1} = x_k - x_{k-1} \quad \text{and} \quad q_{k-1} = (J(x_k) - J(x_{k-1}))^T r(x_k),$$

based on the first order approximation to the Taylor series

$$\left(\sum_{j=1}^m r_j(x_k) \nabla^2 r_j(x_k) \right) s_{k-1} \approx (J(x_k) - J(x_{k-1}))^T r(x_k).$$

By using this secant condition, Dennis, Gay and Welsch [4] derived the update for A_k corresponding to the DFP update, and Al-Baali and Fletcher [1] derived the update for A_k corresponding to the BFGS update. Furthermore, in order to follow the good performance of the Gauss-Newton method in the case of zero residual problems, the former used a sizing technique and the latter proposed a hybrid method in which their structured quasi-Newton method was switched to the Gauss-Newton method if needed. Specifically, Dennis et al. proposed the update

$$(1.7) \quad A_k = \beta_{k-1} A_{k-1} + \frac{(q_{k-1} - \beta_{k-1} A_{k-1} s_{k-1}) y_{k-1}^T + y_{k-1} (q_{k-1} - \beta_{k-1} A_{k-1} s_{k-1})^T}{s_{k-1}^T y_{k-1}} - \frac{s_{k-1}^T (q_{k-1} - \beta_{k-1} A_{k-1} s_{k-1})}{(s_{k-1}^T y_{k-1})^2} y_{k-1} y_{k-1}^T$$

with the sizing factor

$$\beta_{k-1} = \min \left(\left| \frac{s_{k-1}^T (J(x_k) - J(x_{k-1}))^T r(x_k)}{s_{k-1}^T A_{k-1} s_{k-1}} \right|, 1 \right).$$

On the other hand, Al-Baali and Fletcher combined the update

$$(1.8) \quad A_k = A_{k-1} - \frac{(J(x_k)^T J(x_k) + A_{k-1}) s_{k-1} s_{k-1}^T (J(x_k)^T J(x_k) + A_{k-1})^T}{s_{k-1}^T (J(x_k)^T J(x_k) + A_{k-1}) s_{k-1}} + \frac{z_{k-1} z_{k-1}^T}{s_{k-1}^T z_{k-1}}$$

and the Gauss-Newton method.

Both the methods perform well in practical computation, but the matrix $J(x_k)^T J(x_k) + A_k$ does not necessarily possess the hereditary positive definiteness when A_k is updated by the preceding formula. Thus it is not guaranteed for the direction d_k in (1.4) to be a descent search direction for $f(x)$. In order to remedy this difficulty, this paper presents a method that preserves the positive definiteness of a Hessian approximation. For this purpose, we derive a general form of symmetric positive definite matrices that satisfy the secant condition and apply this general form to Gauss-Newton method for solving nonlinear least squares problems.

2 A general class of symmetric positive definite matrices

Letting B_+ be an approximation to the Hessian matrix, the secant condition used in secant methods is generally represented by $B_+ s = z$ for vectors s and z . This section presents a general form that satisfies the following condition:

[SSP Condition]

(1) A matrix B_+ satisfies the secant condition

$$(2.1) \quad B_+ s = z$$

for given vectors $s, z \in R^n$ such that $s^T z > 0$.

(2) A matrix B_+ is symmetric.

(3) A matrix B_+ is positive definite. \square

Note that the positivity of $s^T z$ is a necessary condition for B_+ to be positive definite. An approach given here follows the study by Yamaki and Yabe [7]. In order to find a general form that satisfies the SSP condition, we consider the following problem.

[Problem A]

Given vectors $s, z \in R^n$ such that $s^T z > 0$, find $N_+ \in R^{m \times n}$ that satisfies the secant condition

$$N_+^T N_+ s = z,$$

where $n \leq m$. \square

Then following [7], we obtain the following theorem.

Theorem 1 *The matrix N_+ given by*

$$(2.2) \quad N_+ = \frac{uz^T}{\sqrt{s^T z} \|u\|} + \left(I - \frac{\Phi s u^T}{s^T \Phi^T u} \right) \Phi$$

is a general solution to [Problem A], where $\Phi \in R^{m \times n}$ and $u \in R^m$ are any matrix and vector such that $s^T \Phi^T u \neq 0$. \square

Therefore, setting $C = \Phi^T \Phi$, we can get a form of a matrix that satisfies the SSP condition as follows:

$$(2.3) \quad B_+ = C - \frac{C s s^T C}{s^T C s} + \frac{z z^T}{s^T z} + (s^T C s) w w^T,$$

where

$$w = \frac{\Phi^T u}{s^T \Phi^T u} - \frac{C s}{s^T C s} \quad \text{and} \quad C = \Phi^T \Phi.$$

The following theorem guarantees that the preceding result is a general form that satisfies the SSP condition.

Theorem 2 *The matrix B_+ given by (2.3) is a general form that satisfies the SSP condition, where Φ is any column full rank matrix. \square*

In the remainder of this section, from (2.3), we will give a matrix family that corresponds to the Broyden family for secant methods and its factorized form. Recall that the Broyden family is formed by the linear combination of the BFGS and the DFP updates. So following [6], for $\phi \geq 0$, we set

$$(2.4) \quad u = (1 - \sqrt{\phi}) \frac{\Phi s}{s^T C s} + \sqrt{\phi} \frac{(\Phi^T)^\dagger z}{s^T z}.$$

If a matrix Φ is of column full rank, its Moore-Penrose generalized inverse can be formed as $(\Phi^T)^\dagger = \Phi C^{-1}$. Thus we obtain the Broyden-like matrix family and its factorized form as follows:

$$(2.5) \quad B_+^{Broyden} = C - \frac{C s s^T C}{s^T C s} + \frac{z z^T}{s^T z} + \phi (s^T C s) v v^T,$$

where

$$v = \frac{z}{s^T z} - \frac{C s}{s^T C s}$$

and

$$(2.6) \quad N_+^{Broyden} = \Phi + (1 - \sqrt{\phi}) \left(\frac{\Phi s}{s^T C s} \right) (\sqrt{\lambda} z - C s)^T \\ + \sqrt{\phi} \Phi (\sqrt{\lambda} C^{-1} z - s) \left(\frac{z}{s^T z} \right)^T,$$

where $\phi \geq 0$, and

$$\lambda = \left[(1 - \phi) \frac{s^T z}{s^T C s} + \phi \frac{z^T C^{-1} z}{s^T z} \right]^{-1}.$$

Note that the cases $\phi = 0$ and $\phi = 1$ in (2.5) correspond to a BFGS and a DFP updates, respectively.

3 An application of a general form to Gauss-Newton method

In this section, we apply our general form to solving nonlinear least squares problems. As stated in Section 1, the structured quasi-Newton methods are not guaranteed for the direction d_k in (1.4) to be a descent search direction for $f(x)$. In order to remedy this difficulty, we apply a Broyden-like family in (2.5) to the Gauss-Newton method and obtain a method that satisfies the SSP condition. In this case, a generated matrix preserves the positive definiteness and possess the information on the second part of the Hessian matrix $\nabla^2 f(x)$. By doing so, we expect the modified form becomes a better approximation to the Hessian matrix than the matrix $J(x_k)^T J(x_k)$ in the Gauss-Newton method for both of zero and large residual problems. For this purpose, following (1.5), we consider the following secant condition

$$(3.1) \quad B_k s_{k-1} = z_{k-1},$$

with

$$(3.2) \quad z_{k-1} = J(x_k)^T J(x_k) s_{k-1} + (J(x_k) - J(x_{k-1}))^T r(x_k).$$

If the Jacobian matrix $J(x_k)$ is of column full rank, the matrix $J(x_k)^T J(x_k)$ is symmetric positive definite. Thus setting

$$\Phi = J(x_k), \quad s = s_{k-1} \quad \text{and} \quad z = z_{k-1}$$

in (2.5) and (2.6), we obtain a Broyden-type family and its factorized form as follows:

Broyden-type family:

$$(3.3) \quad B_k^{Broyden-type} = J(x_k)^T J(x_k) - \frac{J(x_k)^T J(x_k) s_{k-1} s_{k-1}^T J(x_k)^T J(x_k)}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}} + \frac{z_{k-1} z_{k-1}^T}{s_{k-1}^T z_{k-1}} + \phi_{k-1} (s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}) v_{k-1} v_{k-1}^T,$$

where

$$v_{k-1} = \frac{z_{k-1}}{s_{k-1}^T z_{k-1}} - \frac{J(x_k)^T J(x_k) s_{k-1}}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}}$$

and

$$(3.4) \quad W_+^{Broyden-type} = J(x_k) + (1 - \sqrt{\phi_{k-1}}) \left(\frac{J(x_k) s_{k-1}}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}} \right) (\sqrt{\lambda_{k-1}} z_{k-1} - J(x_k)^T J(x_k) s_{k-1})^T + \sqrt{\phi_{k-1}} J(x_k) (\sqrt{\lambda_{k-1}} (J(x_k)^T J(x_k))^{-1} z_{k-1} - s_{k-1}) \left(\frac{z_{k-1}}{s_{k-1}^T z_{k-1}} \right)^T,$$

where $\phi_{k-1} \geq 0$, and

$$\lambda_{k-1} = \left((1 - \phi_{k-1}) \frac{s_{k-1}^T z_{k-1}}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}} + \phi_{k-1} \frac{z_{k-1}^T (J(x_k)^T J(x_k))^{-1} z_{k-1}}{s_{k-1}^T z_{k-1}} \right)^{-1}.$$

Furthermore, as members of this family, we have a BFGS-type form and a DFP-type form as follows:

BFGS-type form: The case $\phi_{k-1} = 0$ yields

$$(3.5) \quad B_k^{BFGS-type} = J(x_k)^T J(x_k) - \frac{J(x_k)^T J(x_k) s_{k-1} s_{k-1}^T J(x_k)^T J(x_k)}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}} + \frac{z_{k-1} z_{k-1}^T}{s_{k-1}^T z_{k-1}}$$

and

$$L_k^{BFGS-type} = J(x_k) + \left(\frac{J(x_k) s_{k-1}}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}} \right) (\tau_k z_{k-1} - J(x_k)^T J(x_k) s_{k-1})^T,$$

where

$$\tau_k = \sqrt{\frac{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}}{s_{k-1}^T z_{k-1}}}.$$

DFP-type form: The case $\phi_{k-1} = 1$ yields

$$(3.6) \quad B_k^{DFP-type} = J(x_k)^T J(x_k) - \frac{J(x_k)^T J(x_k) s_{k-1} z_{k-1}^T + z_{k-1} s_{k-1}^T J(x_k)^T J(x_k)}{s_{k-1}^T z_{k-1}} \\ + \left(1 + \frac{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}}{s_{k-1}^T z_{k-1}} \right) \frac{z_{k-1} z_{k-1}^T}{s_{k-1}^T z_{k-1}}$$

and

$$L_k^{DFP-type} = J(x_k) + J(x_k) (\tau_k (J(x_k)^T J(x_k))^{-1} z_{k-1} - s_{k-1}) \left(\frac{z_{k-1}}{s_{k-1}^T z_{k-1}} \right)^T,$$

where

$$\tau_k = \sqrt{\frac{s_{k-1}^T z_{k-1}}{z_{k-1}^T (J(x_k)^T J(x_k))^{-1} z_{k-1}}}.$$

Note that the forms (3.5) and (3.6) are respectively the GN-BFGS and the GN-DFP proposed by Al-Baali and Fletcher [1]. In the case where we use the factorized form, the search direction d_k is a solution to the linear system of equations

$$L_k^T L_k d = -J(x_k)^T r(x_k).$$

4 Some properties

The family (3.3) has the following favorable properties:

- (a) Since it satisfies the secant condition (3.1) with (3.2), this method has more information on the Hessian matrix than the Gauss-Newton method.
- (b) If $s_{k-1}^T z_{k-1} > 0$, it preserves the positive definiteness. This implies that the method produces a descent search direction.

- (c) This method is invariant for the scaling such as $\tilde{x} = Mx$ for M nonsingular. In fact, for a linear transformation M , set

$$\tilde{x} = Mx, \quad \tilde{f}(\tilde{x}) = f(x) \quad \text{and} \quad \tilde{r}(\tilde{x}) = r(x).$$

Then we have

$$\begin{aligned} \tilde{J}(\tilde{x}_k) &= J(x_k)M^{-1}, \\ \tilde{s}_k &= Ms_k, \\ \tilde{z}_k &= (M^T)^{-1}z_k, \\ \tilde{v}_{k-1} &= \frac{\tilde{z}_{k-1}}{\tilde{s}_{k-1}^T \tilde{z}_{k-1}} - \frac{\tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k) \tilde{s}_{k-1}}{\tilde{s}_{k-1}^T \tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k) \tilde{s}_{k-1}}. \end{aligned}$$

Since the scaled matrix \tilde{B}_k is written by

$$\begin{aligned} \tilde{B}_k &= \tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k) - \frac{\tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k) \tilde{s}_{k-1} \tilde{s}_{k-1}^T \tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k)}{\tilde{s}_{k-1}^T \tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k) \tilde{s}_{k-1}} + \frac{\tilde{z}_{k-1} \tilde{z}_{k-1}^T}{\tilde{s}_{k-1}^T \tilde{z}_{k-1}} \\ &\quad + \phi_{k-1}(\tilde{s}_{k-1}^T \tilde{J}(\tilde{x}_k)^T \tilde{J}(\tilde{x}_k) \tilde{s}_{k-1}) \tilde{v}_{k-1} \tilde{v}_{k-1}^T \\ &= (M^T)^{-1} J(x_k)^T J(x_k) M^{-1} - \frac{(M^T)^{-1} J(x_k)^T J(x_k) s_{k-1} s_{k-1}^T J(x_k)^T J(x_k) M^{-1}}{s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}} \\ &\quad + \frac{(M^T)^{-1} z_{k-1} z_{k-1}^T M^{-1}}{s_{k-1}^T z_{k-1}} + \phi_{k-1}(s_{k-1}^T J(x_k)^T J(x_k) s_{k-1}) (M^T)^{-1} v_{k-1} v_{k-1}^T M^{-1} \\ &= (M^T)^{-1} B_k M^{-1}, \end{aligned}$$

the linear system of equations

$$\tilde{B}_k \tilde{d} = -\tilde{J}(\tilde{x}_k)^T \tilde{r}(\tilde{x}_k)$$

yields

$$\begin{aligned} \tilde{d}_k &= -\tilde{B}_k^{-1} \tilde{J}(\tilde{x}_k)^T \tilde{r}(\tilde{x}_k) \\ &= -MB_k^{-1}M^T(M^T)^{-1}J(x_k)^T r(x_k) \\ &= Md_k. \end{aligned}$$

This implies

$$\tilde{x}_{k+1} = \tilde{x}_k + \tilde{d}_k = Mx_{k+1}.$$

- (d) If the magnitude of the residual vector $r(x_k)$ is very small, we may regard $z_{k-1} \approx J(x_k)^T J(x_k) s_{k-1}$ and we may have $B_k^{\text{Broyden-type}} \approx J(x_k)^T J(x_k)$. This implies that this method may perform as well as the Gauss-Newton method does in the case of the zero residual problems. So we expect this method has a self-sizing property. \square

For convergence property, Dennis, Sheng and Vu [5] proposed the damped secant condition

$$(4.1) \quad B_k s_{k-1} = z_{k-1}, \quad z_{k-1} = J(x_k)^T J(x_k) s_{k-1} + \gamma_k (J(x_k) - J(x_{k-1}))^T r(x_k)$$

with $0 \leq \gamma_k \leq \min\{1, \|J(x_k)^T r(x_k)\|\}$ instead of the conditions (3.1) and (3.2), and showed local and q-linear convergence of the methods with (3.5) and (3.6) for $f(x)$ convex and moreover, q-quadratic convergence for the zero residual case.

In the properties above, we stated that the condition $s_{k-1}^T z_{k-1} > 0$ yielded the hereditary positive definiteness. The following theorem guarantees there exists a step size α_k such that this condition is satisfied and this was given by Yabe and Yamaki [6].

Theorem 3 Assume that the Hessian metric $\nabla^2 f(x)$ is positive definite in R^n . Then there exists a positive constant α_k^* such that

$$(\alpha d_k)^T (J(x_k + \alpha d_k)^T J(x_k + \alpha d_k)(\alpha d_k) + (J(x_k + \alpha d_k) - J(x_k))^T r(x_k + \alpha d_k)) > 0$$

for $0 < \forall \alpha < \alpha_k^*$. \square

The proof of this theorem can be found in [6].

We stated above the case where the Jacobian matrix $J(x_k)$ is of column full rank. If $J(x_k)$ is not of column full rank, we can no longer use the preceding argument. In this case, we consider the Levenberg-Marquardt modification such that the matrix $J(x_k)^T J(x_k) + \lambda_k I$ is positive definite for some $\lambda_k > 0$, and we can apply a similar approach to the matrix $J(x_k)^T J(x_k) + \lambda_k I$ to obtain a method that satisfies the SSP condition. We can choose a positive number λ_k such that $J(x_k)^T J(x_k) + \lambda_k I$ is positive definite. Thus setting $C = J(x_k)^T J(x_k) + \lambda_k I$ in (2.5), we obtain

Broyden-type family:

$$\begin{aligned} B_k = & J(x_k)^T J(x_k) + \lambda_k I \\ & - \frac{(J(x_k)^T J(x_k) + \lambda_k I)s_{k-1}s_{k-1}^T(J(x_k)^T J(x_k) + \lambda_k I)}{s_{k-1}^T(J(x_k)^T J(x_k) + \lambda_k I)s_{k-1}} + \frac{z_{k-1}z_{k-1}^T}{s_{k-1}^T z_{k-1}} \\ & + \phi_{k-1}(s_{k-1}^T(J(x_k)^T J(x_k) + \lambda_k I)s_{k-1})v_{k-1}v_{k-1}^T, \end{aligned}$$

where

$$v_{k-1} = \frac{z_{k-1}}{s_{k-1}^T z_{k-1}} - \frac{(J(x_k)^T J(x_k) + \lambda_k I)s_{k-1}}{s_{k-1}^T(J(x_k)^T J(x_k) + \lambda_k I)s_{k-1}}.$$

5 Concluding remarks

We have obtained the general form and its factorized form of a matrix satisfying the SSP condition. This may enable us to unify the positive definite secant updates. We don't restrict ourselves to the secant method. We would like to use our form as the transformation of a given symmetric matrix to one satisfying the SSP condition. Standing from this viewpoint, we have given a modification of the Gauss-Newton method for nonlinear least squares problems.

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